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Renormalization Group Analysis of Finite-Size Scaling in the Φ_4^4 Model*

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Abstract

A finite-size scaling theory for the ϕ_4^4 model is derived using renormalization group methods. Particular attention is paid to the partition function zeroes, in terms of which all thermodynamic observables can be expressed. While the leading scaling behaviour is identical to that of mean field theory, there exist multiplicative logarithmic corrections too. A non-perturbative test of these formulae in the form of a high precision Monte Carlo analysis reveals good quantitative agreement with the analytical predictions.

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1 Introduction

Above one dimension, lattice ϕ^4 theory is known to possess a second order phase transition separating an ordered phase from a disordered one. The continuum parameterization of the field theory is defined at this phase transition. There exist rigorous proofs regarding the trivial (Gaussian) and interactive nature of the continuum theory in $d > 4$ and $d < 4$ dimensions respectively [1]. Although a rigorous proof is still lacking, it is believed that in $d = 4$ the theory is also trivial. Nonetheless, the theory may be useful as one with an effective interaction — valid below some momentum cutoff Λ . In this context, triviality of the theory means that the (leading) critical exponents at the phase transition are identical to those of the Gaussian model which describes free bosons. The renormalization group (RG) approach predicts logarithmic violations of the mean field scaling relations in four dimensions [2, 3]. It has been stated [4] that the existence of such logarithmic corrections to any mean field scaling relation implies triviality. Hence the importance of the study of these corrections and the primary motivation for the present work.

The layout of this paper is as follows:

In sect.2 the perturbative RG is applied to the single component ϕ^4 theory, and a finite-size scaling (FSS) theory is developed with particular emphasis on four dimensions. The approach to criticality from within both the symmetric and broken phases is studied.

The lattice version of the model is then discussed in sect.3. The concept of partition function zeroes as an alternative way to view the onset of a phase transition is recalled. Formulae describing the FSS behaviour of these zeroes are derived. These are then used to derive the FSS formulae of thermodynamic functions.

The RG and FSS equations predict logarithmic violations of the mean field theory in four dimensions. These solutions are based on perturbation theory and have to be tested in an independent approach.

In sect.4 details of our numerical simulations are discussed and the results regarding logarithmic scaling corrections presented. These are consistent with our RG predictions. We conclude in sect.5.

We should mention here that some of the background material is not new. It has been included to keep the presentation as self contained as possible. Our treatment of the FSS behaviour of the Lee–Yang zeroes (as

well as the consequent FSS behaviour of the thermodynamic functions) in four dimensions is, however, new. Some of our numerical results on Fisher zeroes have been presented earlier[5].

2 Renormalization group and finite-size scaling

In the single component version of ϕ^4 theory with quadratic composite fields, the Hamiltonian density in d -dimensional Euclidean space-time continuum may be written as [2]

$$\mathcal{H} = \frac{1}{2}(\nabla\phi)^2 + \frac{m_0^2}{2}\phi^2(x) + \frac{g_0}{4!}\phi^4(x) - H(x)\phi(x) - \frac{t(x)}{2}\phi^2(x). \quad (2.1)$$

Here m_0 is the bare mass of the bosons described by the theory, and g_0 is the bare interaction coupling. $H(x)$ and $t(x)$ are the sources for the fields ϕ and the composite ϕ^2 fields respectively. The generating functionals $Z[H, t]$ and $W[H, t]$ are defined by

$$Z[H, t] = e^{W[H, t]} = C \int \prod_x d\phi(x) e^{-\int d^d x \mathcal{H}}, \quad (2.2)$$

and the constant C is chosen such that

$$W[0, 0] = 0. \quad (2.3)$$

The function conjugate to $H(x)$ is

$$M(x, t) = \frac{\delta W[H, t]}{\delta H(x)} = \langle \phi(x) \rangle_{H, t}. \quad (2.4)$$

Then the generating functional $\Gamma[M, t]$ of the one particle irreducible vertex functions is defined through the Legendre transformation

$$\Gamma[M, t] + W[H, t] = \int dx H(x) M(x), \quad (2.5)$$

with

$$H(x, t) = \frac{\delta \Gamma[M, t]}{\delta M(x)}. \quad (2.6)$$

The objects of interest are the Schwinger functions (or correlation functions). Define

$$\Gamma^{(L,N)}[y_1, \dots, y_L; x_1, \dots, x_N; M; t] = \frac{\delta^{L+N} \Gamma[M, t]}{\delta t(y_1) \dots \delta t(y_L) \delta M(x_1) \dots \delta M(x_N)} \quad . \quad (2.7)$$

This is a functional of M and t (it is a function of its remaining arguments).

At some value of the bare mass, the renormalized theory is massless. Setting, then, m_0 to this critical value, and letting $t(x)$ become independent of x , t becomes a measure of the deviation away from the massless theory. If the source H is also independent of x , then the $\Gamma^{(L,N)}$ become functions (rather than functionals) of all their arguments. This is the situation henceforth assumed.

Power counting yields the (primitive) degree of divergence of an individual graph. In less than four dimensions

$$\Gamma^{(0,2)}, \Gamma^{(0,4)} \text{ and } \Gamma^{(1,2)}$$

are divergent. Renormalization of these three functions gives the renormalized mass m_R , the quartic coupling g_R , the field strength renormalization and the composite field strength renormalization ($Z^{\frac{1}{2}}$ and $Z_{(2)}$ respectively). The composite field strength is renormalized by defining $(\phi^2)_R$ as $Z_{(2)} \times (\phi_R)^2$. Thus

$$(\phi^2)_R = \frac{Z_{(2)}}{Z} \phi^2, \quad (2.8)$$

and the divergence of $Z_{(2)}$ renders $(\phi^2)_R$ finite[2].

In four dimensions there appears an additional divergence due to

$$\Gamma^{(2,0)}.$$

The corresponding diagram has no external legs and can never appear as a subdiagram. The renormalization of $\Gamma^{(2,0)}$ is therefore accomplished by subtracting its divergent part. This subtraction does not effect the other $\Gamma^{(L,N)}$. The relationship between the bare and the massless renormalized theory is [2, 3]

$$\Gamma_R^{(L,N)}(q_1, \dots, q_L; p_1, \dots, p_N; g_R, \mu) = \left(\frac{Z_{(2)}}{Z} \right)^L Z^{N/2}$$

$$\times \left\{ \Gamma_{\text{bare}}^{(L,N)}(q_1, \dots, q_L; p_1, \dots, p_N; g_0, \Lambda) - \delta_{L,2} \delta_{N,0} \Gamma_{\text{bare}}^{(2,0)}(q, -q; g_0, \Lambda) \Big|_{q^2 = \frac{4}{3}\mu^2} \right\}, \quad (2.9)$$

in which Λ is the ultra-violet cutoff and μ is an arbitrary non-vanishing mass parameter.

Following the renormalization prescription of [2], one can then proceed to expand around this critical (massless) theory. This allows one to examine the approach to criticality from within both the symmetric and the broken phases.

The renormalization group equations express the invariance of the physics under a rescaling of the mass parameter $\mu \rightarrow \mu(\lambda)$ defined by

$$\mu(\lambda) \equiv \lambda\mu. \quad (2.10)$$

Following [2] one finds the RGE

$$\left[\lambda \frac{\partial}{\partial \lambda} - \frac{N}{2} \eta(g_R(\lambda)) - L \left(\frac{1}{\nu(g_R(\lambda))} - 2 \right) \right] \times \Gamma_R^{(L,N)}(q; p; t(\lambda), M(\lambda), g_R(\lambda), \mu(\lambda)) = \Theta_{L,N}(\lambda) \quad , \quad (2.11)$$

where

$$\Theta_{L,N}(\lambda) = \frac{\delta_{N0}}{(2-L)!} t(\lambda)^{(2-L)} \Upsilon(g_R(\lambda)) \quad (2.12)$$

for $L \leq 2$ and zero otherwise. We will refer to this term as the inhomogeneous term. It comes from the need to (additively) renormalize $\Gamma^{(2,0)}$ in $d = 4$. Since $\Gamma^{(2,0)}$ is not divergent for $d < 4$, the inhomogeneous term in (2.11) does not give rise to any singular contribution there. The flow equations are

$$\begin{aligned} \lambda \frac{d}{d\lambda} g_R(\lambda) &= B(g_R(\lambda)) & \text{with } g_R(1) &= g_R, \\ \frac{\lambda}{t(\lambda)} \frac{dt(\lambda)}{d\lambda} &= 2 - \frac{1}{\nu(g_R(\lambda))} & \text{with } t(1) &= t, \\ \frac{\lambda}{M(\lambda)} \frac{dM(\lambda)}{d\lambda} &= -\frac{1}{2} \eta(g_R(\lambda)) & \text{with } M(1) &= M \end{aligned} \quad (2.13)$$

and

$$\Upsilon(g_R) = \left[2 \left(\frac{1}{\nu(g_R)} - 2 \right) - \mu \frac{d}{d\mu} \right] \left(\frac{Z_{(2)}}{Z} \right)^2 \Gamma_{\text{bare}}^{(2,0)}(q, -q; g_0, \Lambda) \Big|_{q^2 = \frac{4}{3}\mu^2}. \quad (2.14)$$

The content of the RGE (2.11) is, then, that if μ is rescaled by a factor λ then the response of g_R , t and M is governed by (2.13).

The Callan Symanzik beta function [6] is denoted by B in (2.13). The form of this function can be calculated perturbatively in the renormalized $d = (4 - \epsilon)$ dimensional theory. Eq.(2.13) then gives the behaviour of the running coupling constant $g_R(\lambda)$. It turns out that in order to remove the cutoff, the running coupling constant $g_R(\lambda)$ has to approach the infra-red (IR) fixed point $g_R^* \sim O(\epsilon)$. This fixed point then governs the critical region.

The region of interest can be divided into

(a) $t \geq 0$, $H = 0$. In this region there is no magnetization ($M = 0$). This is a symmetric theory.

(b) $t > 0$ and $H \neq 0$ or $t < 0$ and any H . This is the region of broken symmetry (in which $M \neq 0$).

The RGE (2.11) holds throughout regions (a) and (b). The point in using vertex functions is that it is nowhere necessary to state whether or not the symmetry is broken (be it spontaneously or explicitly) [7].

The solution of (2.11) is

$$\begin{aligned} \Gamma_R^{(L,N)}(q; p; t, M, g_R, \mu) &= \tilde{Z}(\lambda, g_R(\lambda)) \\ &\times \Gamma_R^{(L,N)}(q; p; t(\lambda), M(\lambda), g_R(\lambda), \mu(\lambda)) + \Pi_{L,N}(\lambda), \end{aligned} \quad (2.15)$$

where

$$\begin{aligned} \tilde{Z}(\lambda, g_R(\lambda)) &= e^{-\int_{g_R}^{g_R(\lambda)} \left[\frac{N}{2} \eta(g_R) + L \left(\frac{1}{\nu(g_R)} - 2 \right) \right] \frac{dg_R}{B(g_R)}} \\ &= \left(\frac{M(\lambda)}{M} \right)^N \left(\frac{t(\lambda)}{t} \right)^L, \end{aligned} \quad (2.16)$$

and the inhomogeneous term is

$$\Pi_{L,N}(\lambda) = \int_1^\lambda \frac{d\lambda'}{\lambda'} \Theta_{L,N}(\lambda') \tilde{Z}(\lambda', g_R(\lambda')). \quad (2.17)$$

Because of the local nature of the RG, the renormalization constants of the infinite volume theory render finite the finite volume theory too [8, 9]. We denote by $\Gamma_R^{(L,N)}(q; p; t, M, g_R, \mu, l)$ the renormalized Schwinger function of the finite volume theory, where l denotes the linear extent of the system. The

RGE obeyed by this Schwinger function is the same as (2.11). Its solution is (from (2.15))

$$\begin{aligned}\Gamma_R^{(L,N)}(q; p; t, M, g_R, \mu, l) &= \tilde{Z}(\lambda, g_R(\lambda)) \\ &\times \Gamma_R^{(L,N)}(q; p; t(\lambda), M(\lambda), g_R(\lambda), \mu\lambda, l) + \Pi_{L,N}(\lambda).\end{aligned}\quad (2.18)$$

To prepare for dimensional analysis, we implicitly replace g_R by $\mu^\epsilon g_R$ to keep it dimensionless. Then applying dimensional analysis to the homogeneous term on the right hand side gives

$$\begin{aligned}\Gamma_R^{(L,N)}(q; p; t, M, g_R, \mu, l) &= \tilde{Z}(\lambda, g_R(\lambda)) l^{\frac{N}{2}(d-2)+2L-d} \\ &\times \Gamma_R^{(L,N)}(lq; lp; l^2 t(\lambda), l^{\frac{d-2}{2}} M(\lambda), g_R(\lambda), l\mu\lambda, 1) + \Pi_{L,N}(\lambda).\end{aligned}\quad (2.19)$$

Since λ is still at our disposal (as long as it is small enough so as to remain in the critical region), we choose

$$l\mu\lambda = 1. \quad (2.20)$$

Then,

$$\begin{aligned}\Gamma_R^{(L,N)}(q; p; t, M, g_R, \mu, l) &= \left(\frac{M(1/l\mu)}{M}\right)^N \left(\frac{t(1/l\mu)}{t}\right)^L l^{\frac{N}{2}(d-2)+2L-d} \\ &\times \Gamma_R^{(L,N)}\left(lq; lp; l^2 t \left(\frac{1}{l\mu}\right), l^{\frac{d-2}{2}} M\left(\frac{1}{l\mu}\right), g_R\left(\frac{1}{l\mu}\right), 1, 1\right) \\ &+ \Pi_{L,N}\left(\frac{1}{l\mu}\right).\end{aligned}\quad (2.21)$$

In less than four dimensions, and in the critical region, the flow equations give [2, 8]

$$t(\lambda) = t\lambda^{(2-\frac{1}{\nu})} \quad (2.22)$$

$$M(\lambda) = M\lambda^{-\frac{1}{2}\eta}. \quad (2.23)$$

If $l\mu$ is large enough then $g_R(\frac{1}{l\mu})$ is close to g_R^* . Therefore, at zero momentum,

$$\begin{aligned}\Gamma_R^{(L,N)}(0; 0; t, M, g_R, \mu, l) &= \mu^{\frac{N}{2}\eta+L(\frac{1}{\nu}-2)} l^{\frac{N\beta}{\nu}+\frac{L}{\nu}-d} \\ &\times \Gamma_R^{(L,N)}\left(0; 0; \mu^{\frac{1}{\nu}-2} l^{\frac{1}{\nu}} t, \mu^{\frac{1}{2}\eta} l^{\frac{\beta}{\nu}} M, g_R^*, 1, 1\right) + \Pi_{L,N}\left(\frac{1}{l\mu}\right),\end{aligned}\quad (2.24)$$

where

$$\beta = \frac{\nu}{2}(d - 2 + \eta). \quad (2.25)$$

If μ is fixed, then

$$\Gamma_R^{(L,N)}(0; 0; t, M, g_R, \mu, l) = l^{\frac{N\beta}{\nu} + \frac{L}{\nu} - d} F_\mu^{(L,N)} \left(l^{\frac{1}{\nu}} t, l^{\frac{\beta}{\nu}} M \right) + \Pi_{L,N} \left(\frac{1}{l\mu} \right), \quad (2.26)$$

where $F_\mu^{(L,N)}$ is an unknown function of its arguments. Eq.(2.6) can be applied to this form for $\Gamma_R^{(0,0)}$ to express the external field H in terms of M . This gives

$$\Gamma_R^{(L,N)}(0; 0; t, H, g_R, \mu, l) = l^{\frac{N\beta}{\nu} + \frac{L}{\nu} - d} F_\mu'^{(L,N)} \left(l^{\frac{1}{\nu}} t, l^{\frac{\delta\beta}{\nu}} H \right) + \Pi_{L,N} \left(\frac{1}{l\mu} \right). \quad (2.27)$$

Here δ is the usual odd critical exponent defined by

$$\delta = \frac{d + 2 - \eta}{d - 2 + \eta}. \quad (2.28)$$

Eq.(2.27) is sufficient to derive the usual FSS relations in less than four dimensions [10, 8, 11].

For example, the zero field susceptibility is given by

$$\chi_l^{-1}(t) = \Gamma_l^{(0,2)}(0; t, 0, g_R, \mu) = l^{\frac{2\beta}{\nu} - d} F_\chi(l^{\frac{1}{\nu}} t),$$

where F_χ is, again, an unknown function. Putting $t = 0$ then gives the FSS behaviour of the zero field susceptibility at the infinite volume critical point, $\chi_l(t = 0) \propto l^{2-\eta}$.

In the four dimensional version of the theory there appear certain subtleties which are not present below four dimensions. This is because the IR fixed point of the Callan-Symanzik function $B(g_R)$ moves to the origin as the dimension becomes four. Secondly, in contrast to the $d < 4$ dimensional case, the fixed point is now a double zero, responsible for the occurrence of logarithmic corrections.

A third difference between the cases of $d < 4$ and $d = 4$ comes from the inhomogeneous term in the RGE. The graph responsible for this term is not in fact divergent when $d < 4$. Singular behaviour in less than four dimensions comes from the homogeneous term. In $d = 4$ the inhomogeneous

term contributes to the leading singular behaviour too. The first term remains singular however, and is responsible for divergences such as that in the susceptibility.

Eq.(2.27), from which the FSS behaviour of the model can be derived below four dimensions, was established with the help of the approximation $g_R(\frac{1}{\mu l}) \simeq g_R^*$ for large μl . As pointed out by Brézin in [8], this approximation fails in four dimensions. The reason is that g_R^* then becomes zero, and one is left with the mean field theory.

In $d = 4$, we then have to rely on a perturbative expansion in g_R . To lowest order, the functions $B(g_R)$, $\eta(g_R)$, $\nu(g_R)$ and $\Upsilon(g_R)$ are [2, 3]

$$B(g_R) = \frac{3}{2}g_R^2 - \frac{17}{12}g_R^3 + O(g_R^4), \quad (2.29)$$

$$\eta(g_R) = \frac{1}{24}g_R^2 + O(g_R^3), \quad (2.30)$$

$$\frac{1}{\nu(g_R)} = 2 - \frac{1}{2}g_R + O(g_R^3), \quad (2.31)$$

$$\Upsilon(g_R) = \frac{1}{2} + O(g_R). \quad (2.32)$$

Putting $\mu = 1$ for simplicity, these perturbative solutions, together with the flow equations (2.13), give for (2.21)

$$\begin{aligned} \Gamma_R^{(L,N)}(q; p; t, M, g_R, 1, l) &\simeq \left(\frac{2}{3g_R \ln l} \right)^{L/3} l^{N+2L-4} \\ &\times \Gamma_R^{(L,N)} \left(lq; lp; l^2 t \left(\frac{2}{3g_R \ln l} \right)^{1/3}, lM, \frac{2}{3 \ln l}, 1, 1 \right) \\ &+ \frac{\delta_{N0}}{(2-L)!} \frac{3}{2} \left(\frac{2}{3g_R} \right)^{2/3} t^{2-L} (\ln l)^{1/3}. \end{aligned} \quad (2.33)$$

The coupling constant for the Schwinger function on the right hand side is $\frac{2}{3 \ln l}$ for large l . Since this is small, perturbation theory may be applied to calculate $\Gamma_R^{(0,0)}$ [2]. This gives

$$\begin{aligned} \Gamma_R^{(0,0)}(t, M, g_R, 1, l) \\ = c_1 t M^2 (\ln l)^{-1/3} + c_2 M^4 (\ln l)^{-1} + c_3 t^2 (\ln l)^{1/3} \end{aligned} \quad (2.34)$$

where c_1, c_2 and c_3 are constants. Applying (2.6) to this yields for the external field

$$H(t, M, g_R, 1, l) \simeq c_4 t M (\ln l)^{-1/3} + c_5 M^3 (\ln l)^{-1}, \quad (2.35)$$

where, again, c_4 and c_5 are constants.

The free energy per unit volume in the presence of an external field is

$$W_l(t, H) = MH(t, M; l) - \Gamma_R^{(0,0)}(t, M; l). \quad (2.36)$$

Eqs.(2.35) and (2.34) give, then,

$$W_l(t, H) = c'_1 \frac{tM^2}{(\ln l)^{1/3}} + c'_2 \frac{M^4}{\ln l} + c_3 t^2 (\ln l)^{1/3}, \quad (2.37)$$

where c'_1 and c'_2 are constants and M is related to H through (2.35). This expression is the basis of all the FSS relations derived below.

If H vanishes, then all of the solutions of (2.35) lead to

$$W_l(t, 0) \propto t^2 (\ln l)^{\frac{1}{3}}. \quad (2.38)$$

3 Lattice ϕ^4 theory and the zeroes of the partition function

Within the path integral formulation of quantum field theory there are two complimentary approaches. The first is perturbation theory (in the quartic coupling g_R). Indeed this is the basis for the considerations at the end of the previous section. The second approach is intrinsically non-perturbative. It involves the use of stochastic techniques to calculate the path integrals. Apart from statistical errors numerical approaches are exact, but limited to finite lattice volumes.

We have used such a numerical approach — the Monte Carlo (MC) method — to further study the logarithmic corrections involved in four dimensions. In particular, we present numerical evidence of the validity of the FSS formulae presented in the last section. Thus we have two independent approaches, whose agreement leaves little doubt that this FSS analysis indeed correct. This provides support for the validity of the analyses presented in [2],[3] and [8], and for the triviality of ϕ_4^4 theory.

The usual regularization for a numerical approach replaces the space-time continuum by a lattice. This is, of course, entirely equivalent to the use of the momentum cut-off in sect.2. We use a regular hypercubic lattice of unit intersite spacing. If t is independent of x in (2.1), the lattice parameterized action in the absence of a source field and with finite differences replacing derivatives reads

$$- \kappa \sum_{x,\mu} \phi_x \phi_{x+\mu} + \sum_x \phi_x^2 + \lambda \sum_x (\phi_x^2 - 1)^2 \quad . \quad (3.1)$$

Here the hopping parameter κ and the quartic coefficient λ correspond, in a sense, to the mass and quartic coupling of the continuum theory respectively. Taking λ to infinity gives the Ising limit of the model. Here, the fields ϕ_x take only values from the set $\{\pm 1\}$. The universality hypothesis, which comes from experience in statistical physics, implies that no information should be lost in going to the Ising extreme. I.e., the Ising model and the ϕ^4 model with arbitrary κ and λ should be in the same universality class and exhibit the same scaling behaviour (for a related MCRG study cf.[12]). The vacuum to vacuum transition amplitude of the quantum field theory becomes the partition function of the Ising model.

In the presence of an external field the Ising model can be defined by the partition function

$$Z(\kappa, H) = \frac{1}{\mathcal{N}} \sum_{\{\phi\}} e^{\kappa S + h M} \quad (3.2)$$

where

$$S = \sum_x \sum_{\mu=1}^d \phi_x \phi_{x+\mu} \quad , \quad M = \sum_x \phi_x \quad . \quad (3.3)$$

Here, the Boltzmann factor has been absorbed into the hopping parameter κ , and into the reduced external field $h = \kappa \times H$. The sum runs over all \mathcal{N} possible configurations of the spin field on the d dimensional lattice, and the normalization ensures $Z(0, 0) = 1$. We may reexpress the partition function by

$$\begin{aligned} Z(\kappa, h) &= \sum_{M=-N}^N \sum_{S=-dN}^{dN} \rho(S, M) e^{\kappa S + h M} \\ &= \sum_{M=-N}^N \rho(\kappa; M) e^{h M} = \sum_{S=-dN}^{dN} \rho(S; h) e^{\kappa S} \quad , \end{aligned} \quad (3.4)$$

where N is the number of sites on the lattice. The spectral density $\rho(S, M)$ denotes the relative weight of configurations having given values of S and M . By $\rho(\kappa; M)$ and $\rho(S; h)$ we denote the correspondingly integrated densities.

Z is a polynomial in the fugacity e^{2h} (degree N) and $e^{4\kappa}$ (degree $dN/2$). The coefficients of the polynomial in e^{2h} for real constant κ are real and positive, as are those of the polynomial in $e^{4\kappa}$ for real constant h . A knowledge of the zeroes of the partition function is equivalent to a knowledge of Z itself (and of all functions derivable from it). In particular, the critical behaviour of Ising-type systems can be analysed through its partition function zeroes instead of more traditional methods involving real parameters.

The study of partition function zeroes in general was initiated by Yang and Lee in 1952 [13]. The Lee–Yang theorem states that for ferromagnetic systems all of the zeroes of the partition function in the external ordering magnetic field variable lie on the imaginary axis for real temperatures. Fisher was the first to analyse the zeroes in the complex temperature (or mass) plane [14]. Thus we refer to partition function zeroes in the temperature plane as Fisher zeroes and to those in the complex plane of external fields as Lee–Yang zeroes. With the exception of systems which are self dual [15], there exist no simple general results of the Lee–Yang type concerning the locus of Fisher zeroes. Thus the vast majority of studies have been of a numerical nature (see, however [16, 17] and references therein).

Itzykson, Pearson and Zuber [18] initiated the study of FSS of partition function zeroes. Their analysis was confined to less than four dimensions with power-law scaling behaviour and corrections. This was later extended to dimensions above (not including) four in [19]. The latter is also restricted to purely power-law scaling behaviour. In this section, the corresponding FSS theory is presented for four dimensions where logarithmic corrections are manifest.

Denote by $C_l(t)$ and $\chi_l(t)$ the specific heat and magnetic susceptibility (per unit volume) respectively of a system of linear extent l and at a reduced temperature t in zero external magnetic field (cf. sect.3). Twice differentiating the free energy in the perturbative RG formula (2.38) gives

$$C_l(t) \propto (\ln l)^{\frac{1}{3}}. \quad (3.5)$$

The total free energy at the critical temperature in four dimensions in

the presence of an external field is given by (2.37) as

$$l^4(\ln l)^{\frac{1}{3}}H^{\frac{4}{3}}. \quad (3.6)$$

The partition function is therefore

$$Z_l(t=0, H) = Q\left(l^4(\ln l)^{\frac{1}{3}}H^{\frac{4}{3}}\right). \quad (3.7)$$

If at some (complex) value of H the partition function vanishes, then, for this value of H ,

$$H^{\frac{4}{3}} = l^{-4}(\ln l)^{-\frac{1}{3}}Q^{-1}(0). \quad (3.8)$$

Therefore

$$H_j \propto l^{-3}(\ln l)^{-\frac{1}{4}} \quad (3.9)$$

where the constant of proportionality depends on the index j of the zero. This is the FSS formula for Lee–Yang zeroes in four dimensions.

Eq.(2.38) gives for the total free energy (when $H = 0$)

$$F_l(t, H=0) \propto l^4 t^2 (\ln t)^{\frac{1}{3}}. \quad (3.10)$$

The partition function is the exponential of this, i.e.,

$$Z_l(t, H=0) = R\left(l^4 t^2 (\ln t)^{1/3}\right). \quad (3.11)$$

If R vanishes, then,

$$t^2 l^4 (\ln t)^{1/3} = R_j^{-1}(0) \quad (3.12)$$

where j indicates the index of the zero. Therefore, for the j^{th} zero,

$$t_j \propto l^{-2} (\ln l)^{-1/6} \quad (3.13)$$

where the proportionality constant depends, again, on j .

The scaling relations for the partition function zeroes can be used to find the behaviour of the thermodynamic functions as well. The partition function is a polynomial and as such can be written in terms of its zeroes. Let H_j be the j^{th} Lee–Yang zero for a system of linear extent l . Then, the partition function is

$$Z_l(\kappa, H) \propto \prod_j (H - H_j). \quad (3.14)$$

The magnetic susceptibility is given by the second derivative of the Gibbs free energy with respect to H . This gives, in $d = 4$,

$$\chi_l(\kappa, H) \propto \frac{1}{l^4} \sum_j \frac{1}{(H - H_j)^2}. \quad (3.15)$$

Therefore the susceptibility at the critical value of H (namely at $H = 0$) is

$$\chi_l(\kappa, 0) \propto \frac{1}{l^4} \sum_j \frac{1}{H_j^2}. \quad (3.16)$$

Eq.(3.9) then gives the FSS formula for the zero field susceptibility in four dimensions as

$$\chi_l(\kappa_c, H = 0) \propto l^2 (\ln l)^{\frac{1}{2}}. \quad (3.17)$$

A similar calculation for the Fisher zeroes leads to the recovery of the FSS formula for specific heat (3.5). Let κ_j be the j^{th} Fisher zero for a system of linear extent l . Then, in zero field, the partition function is

$$Z_l(\kappa) \propto \prod_j (\kappa - \kappa_j). \quad (3.18)$$

The specific heat is given by the second derivative of the free energy with respect to t . This gives, in $d = 4$,

$$C_l(\kappa) = -\frac{1}{l^4} \sum_j \frac{1}{(\kappa - \kappa_j)^2}. \quad (3.19)$$

Therefore the specific heat at the critical value of κ is

$$C_l(\kappa_c) = -\frac{1}{l^4} \sum_j \frac{1}{\tau_j^2} \quad (3.20)$$

where τ_j is the ‘reduced’ position of the j^{th} zero:

$$\tau_j = \kappa_j - \kappa_c. \quad (3.21)$$

Eq.(3.13) gives

$$\tau_j \propto l^{-2} (\ln l)^{-\frac{1}{6}} \quad (3.22)$$

where the constant of proportionality depends on the index j . Thus the FSS formula for the specific heat in four dimensions is [20]

$$C_l(\kappa_c) \propto (\ln l)^{\frac{1}{3}}. \quad (3.23)$$

The partition function zeroes provide an alternative way to view the onset of criticality. As the system size increases towards infinity, the zeroes tend to pinch the real H or κ axes ((3.9) and (3.13)). Thermodynamic observables such as the specific heat and magnetic susceptibility become divergent. This applies to the correlation length as well. The FSS formula for the correlation length of a four dimensional system also involves logarithmic corrections. This was derived by Brézin [8] for a system of extent l in all directions. At the infinite volume critical point $\kappa = \kappa_c$, one has

$$\xi_l(\kappa_c) \propto l(\ln l)^{\frac{1}{4}} \quad (3.24)$$

This suggests that a FSS variable should indeed be defined by

$$\frac{\xi_\infty(\kappa)}{\xi_l(\kappa_c)} = \frac{t^{-\frac{1}{2}} |\ln t|^{\frac{1}{6}}}{l(\ln l)^{\frac{1}{4}}} \quad (3.25)$$

in four dimensions[5].

4 Numerical calculations and results

We now want to report on our numerical calculations which confirm the scaling picture of sect.2. In particular, we want to identify the multiplicative logarithmic corrections to FSS. Such logarithmic corrections have been notoriously difficult to verify numerically (see e.g. [4] and [20]). However, the advent of more efficient cluster algorithms [21, 22] has greatly improved the quality of Monte Carlo calculations for bosonic spin systems like the Ising model. We suggest — and the quality of our results supports our proposal — that a study of the FSS of partition function zeroes lends itself more readily to the detection of logarithms than do the more traditional thermodynamic quantities such as specific heat.

The first numerical calculations of partition function zeroes appeared in the 1960's [23]. Such early work involved exact calculations of the density of

states (spectral density) $\rho(S, M)$ and were therefore confined to very small lattices. (See [24] for a list of references and early history).

The next major step concerning numerical calculations was made by Falcioni et al.[25] and by Marinari et al.[26] in the early 1980's. They were the first to use approximations to the density of states in the form of histograms to study critical phenomena. It is clear that straightforward analytical continuation can take (3.4) to the complex κ or H plane. Thus the histogram technique can be used for a precise numerical determination of the complex partition function zeroes.

Numerical methods received a further boost with the development of techniques whereby a number of Monte Carlo constructed histograms can be combined to form one 'multihistogram' [27, 28]. These provide a better approximation to the spectral density over a wider range of the parameter κ or H .

We now present some details of our own numerical calculations. The data were taken on lattices of size from 8^4 to 24^4 using the Swendsen–Wang cluster algorithm. Histograms were determined at $h = 0$ and at various values of κ close to the pseudocritical one (chosen to be that value of κ where the specific heat peaks). Table 1 provides a list of lattices sizes, the values of κ at which the simulations took place, as well as a summary of the statistics.

For the determination of $\rho(S; h = 0)$ the various 'raw' histograms were suitably combined following [27]; no binning was used. With (3.4) this allows one to construct $Z(\kappa, h = 0)$ in the complex neighbourhood of the real κ -values and to determine nearby Fisher zeroes.

For $\rho(\kappa; M)$ we binned each of the raw (S, M) -histograms in a 256×256 array and then combined for each M -bin the corresponding S -subhistograms according [27]. This then allows us to obtain an optimal $\rho(\kappa_0; M)$ for arbitrary κ_0 in the considered domain. From this $Z(\kappa_0, h)$ may be determined for not too large values of (imaginary) h . Below we present results for Lee–Yang zeroes evaluated at $\kappa_0 = \kappa_c$. As a consistency check we also determined the zeroes coming from a single M -histogram corresponding to a simulation at κ_c .

The errors in the quantities calculated from the multihistograms were estimated by the jackknife method, i.e. the data for each lattice size were cut to produce 10 subsamples leading to different multihistograms and thus to different results, whence the variance and bias were calculated [29].

From the Lee–Yang theorem [13] it is known that the zeroes in H all lie on

the imaginary axis for any lattice size l . The search for the Lee–Yang zeroes is therefore technically easier than for the Fisher zeroes. In the later case we used a Newton–Raphson type algorithm. In order to avoid instabilities due to the large numbers involved, and since $Z_l(\kappa)$ never vanishes for real κ , the Fisher zeroes were in fact found as local steep minima in $|Z_l(\kappa)/Z_l(\text{Re } \kappa)|^2$.

We now come to the FSS analysis of the Fisher zeroes. The positions of the closest two Fisher zeroes obtained from the multihistograms are listed in table 2 (where κ_j represents the j^{th} Fisher zero). Since we can confine the scaling analysis to the imaginary parts of the zeroes we avoid the necessity of knowing the infinite volume critical value of κ . In fig.1a we plot the logarithm of the imaginary part of the position of the first Fisher zero against the logarithm of the lattice size l . A linear fit to the slope $(-\frac{1}{\nu})$ gives $\nu = 0.479(1)$ which is slightly below the mean field value of $\frac{1}{2}$. This deviation from the mean field value is due to the presence of logarithmic corrections, which we have neglected in this first fit. A corresponding analysis applied to the second Fisher zeroes gives $\nu = 0.467(8)$.

Assuming that the leading scaling behaviour is indeed proportional to l^2 , we can proceed to search for multiplicative logarithmic corrections. To this end, we plot in fig.1b $\ln(l^2 \text{Im} \kappa_1)$ versus $\ln(\ln l)$. A negative slope is clearly identified and is in good agreement with the scaling prediction of $-\frac{1}{6}$. In fact, a fit to all five points gives a slope $-0.217(12)$. Excluding the point corresponding to $l = 8$ gives a slope of $-0.21(4)$. The solid line is the best fit to the points corresponding to $l = 12 \dots 24$ assuming the theoretical prediction $-\frac{1}{6}$ from (3.13).

The errors in the second (and higher index) Fisher zeroes are too large to warrant a corresponding analysis.

Now that the logarithmic corrections to the FSS behaviour of the Fisher zeroes have been established, we may proceed to determine the infinite volume critical hopping parameter κ_c from

$$|\kappa_j - \kappa_c| \propto l^{-2} (\ln l)^{-\frac{1}{6}}. \quad (4.1)$$

Using the first Fisher zeroes, we find $\kappa_c \simeq 0.149703(15)$ in good agreement with the value $0.149668(30)$ from high temperature expansions [30].

Mean field theory [18] predicts that the angle φ at which the Fisher zeroes depart from the real axis should be $\frac{\pi}{4}$. There exists, unfortunately, no FSS theory for this quantity. We list, in table 3, our measurements of this angle

defined by the first and second Fisher zeroes and the real axis for the five lattice sizes analysed and plot it in fig.2. The average value compares well with the mean field prediction.

Let us now discuss the results for the Lee–Yang zeroes. For all real κ they have to lie on the imaginary h -axis. At κ_c they should scale according to the FSS formula (3.9). Table 4 lists the positions of the first two Lee–Yang zeroes as obtained from the multihistogram at $\kappa_c = 0.149703$. Fig.3a is a log-log plot of the imaginary parts of the positions of the first Lee–Yang zeroes against the lattice size. The resulting slope is $-3.083(4)$; this compares well with mean field prediction of -3 . The deviation, again, may be explained by logarithmic corrections.

To identify the logarithmic corrections, we plot in fig.3b $\ln(l^3 \text{Im} h_1)$ against $\ln(\ln l)$. For the first Lee–Yang zeroes a best fit to all five points gives a slope of $-0.204(9)$ which compares well with the theoretical prediction of $-\frac{1}{4}$ from (3.9). Excluding the smallest lattice, a best fit to the remaining four points gives a slope $-0.22(3)$. The solid line in fig.3b is the best fit to the last four point with given slope $-\frac{1}{4}$.

The errors in the positions of the second nearest Lee–Yang zeroes are only about twice that of the corresponding first index zeroes and these can also be used to analyse FSS. The results again are good agreement with the expected scaling behaviour.

5 Conclusions

We have used RG techniques to derive the FSS behaviour of the ϕ^4 theory in $d=4$, placing particular emphasis on the partition function zeroes. These formulae were then tested in a non-perturbative fashion — with high precision numerical methods. Of primary interest are the multiplicative logarithmic corrections to the leading power law scaling behaviour. These logarithmic corrections are clearly identified from the scaling behaviour of the closest Fisher and Lee–Yang zeroes and are in good quantitative agreement with the theory. Higher index partition function zeroes and thermodynamic observables such as the specific heat exhibit logarithmic corrections too.

The high precision of the numerical results and the good quantitative agreement with the analytical predictions of sect.3 provide non-perturbative evidence for the existence of a double zero in the Callan-Symanzik beta

function. The fixed point responsible for non-trivial behaviour in $d < 4$ dimensions has moved to the position of the trivial fixed point in $d=4$. The results support the assertion that ϕ^4 theory is trivial in four dimensions.

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Tables

Table 1: For each lattice size L we list the values of κ at which MC simulations were performed. The corresponding h value is always zero. In parentheses we give the number of measurements in units of 1000 ($\#/1000$).

L	$\kappa_0(\# /1000)$			
8	0.149709 (400), 0.1525 (400), 0.1533 (400),	0.1506 (200), 0.1527 (400), 0.1540 (200)	0.1515 (200), 0.1529 (400),	0.1520 (200), 0.1531 (400),
12	0.149709 (200), 0.1510 (200),	0.1498 (100), 0.1512 (200),	0.1503 (100), 0.1514 (200),	0.1508 (200), 0.1520 (100)
16	0.1492 (50), 0.1503 (100), 0.1506 (150), 0.1518 (50)	0.1496 (50), 0.1504 (100), 0.1509 (100),	0.149709 (150), 0.1505 (150), 0.1511 (50),	0.1500 (50), 0.15054 (150), 0.1513 (50),
20	0.1495 (30), 0.1500 (50), 0.1504 (50),	0.149709 (80), 0.1501 (100), 0.1507 (30)	0.1498 (30), 0.1502 (80),	0.1499 (50), 0.1503 (80),
24	0.1495 (20), 0.1500 (80),	0.149709 (80), 0.1501 (80),	0.1498 (108), 0.1502 (80),	0.1499 (68), 0.1504 (20)

Table 2: The positions of the first and second Fisher zeroes as obtained from the jackknifed multi-histograms.

L	$\text{Re}(\kappa_1)$	$\text{Im}(\kappa_1)$	$\text{Re}(\kappa_2)$	$\text{Im}(\kappa_2)$
8	0.152156(10)	0.004046(10)	0.154195(104)	0.006085(127)
12	0.150802(7)	0.001733(10)	0.151652(86)	0.002615(137)
16	0.150322(7)	0.000948(5)	0.150913(38)	0.001352(41)
20	0.150095(5)	0.000595(7)	0.150397(55)	0.000875(36)
24	0.149972(3)	0.000414(5)	0.150198(40)	0.000574(48)

Table 3: The angle $\varphi_{1,2}$ between the first and second Fisher zeroes as obtained from the jackknifed multi-histograms. Mean field theory predicts $\varphi = \pi/4 \simeq 0.785$.

L	$\varphi_{1,2}$
8	0.785(62)
12	0.804(139)
16	0.599(89)
20	0.747(175)
24	0.617(246)
mean	0.731(45)

Table 4: The positions of the first two Lee–Yang zeroes as obtained from the jackknifed multihistograms at $\kappa = 0.149703$. The real part of the zeroes is always zero.

L	$\text{Im}(h_1)$	$\text{Im}(h_2)$
8	0.0022294(32)	0.0049488(71)
12	0.0006367(23)	0.0014111(22)
16	0.0002637(9)	0.0005845(33)
20	0.0001327(7)	0.0002949(18)
24	0.0000749(5)	0.0001656(7)

Figures

Fig. 1: (a) The imaginary part of the Fisher zeroes closest to the real κ axis vs. the logarithm of the lattice size L . The straight line is a fit to all points with slope $-2.088(6)$, slightly differing from the expected value $-1/\nu = -2$. This difference is due to logarithmic corrections to scaling as shown in (b), where we plot $\ln(L^2 \text{Im}\kappa_1)$ vs. $\ln \ln L$.

Fig. 2: The impact angle $\varphi_{1,2}$ of the closest two Fisher zeroes, compatible with the expected value $\pi/2$ (full line) within the error (shaded area).

Fig. 3: (a) The imaginary part of the Lee–Yang zeroes closest to $h = 0$ vs. the logarithm of the lattice size, for $\kappa = 0.149703$. The straight line is a fit to all points with slope $-3.083(4)$, slightly differing from the expected value $-1/\delta = -3$. This difference is due to logarithmic corrections to scaling as shown in (b), where we plot $\ln(L^3 \text{Im}h_1)$ vs. $\ln \ln L$.